On a 3d magnetic Hamiltonian with axisymmetric potential and unitary magnetic field

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ON A 3D MAGNETIC HAMILTONIAN WITH AXISYMMETRIC POTENTIAL AND UNITARY MAGNETIC FIELD

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ABSTRACT. This study is about a magnetic Hamiltonian with axisymmetric potential in $\mathbb{R}^3$. The associated magnetic field is planar, unitary and non-constant. The problem reduces to a 1D family of singular Sturm-Liouville operators on the half-line. We study the associated band functions, in particular their behavior at infinity and we describe the quantum state localized in energy near the Landau levels that play the role of threshold in the spectrum. We compare our Hamiltonian to the "de Gennes" operators arising in the study of a 2D Hamiltonian with monodimensional, odd and discontinuous magnetic field. We show in particular that the ground state energy is higher in dimension 3.

1. INTRODUCTION

1.1. **Quantum transport in translationally invariant magnetic systems.** The motion of a spinless quantum particle in $\mathbb{R}^n$ (here $n = 2, 3$) moving in a magnetic field $\mathbf{B}$ is well described by the spectral properties of the associated Hamiltonian, namely the magnetic Laplacian $H_{\mathbf{A}} := (-i\nabla - \mathbf{A})^2$ acting on $L^2(\mathbb{R}^n)$, where $\mathbf{A}$ is a magnetic potential satisfying $\operatorname{curl} \mathbf{A} = \mathbf{B}$. As in the classical picture, we expect the variation of the magnetic field to induce transport for a quantum particle, a well-known phenomenon when adding a boundary to a system with constant magnetic field (in this case edge currents appears along the boundary and are at the core of the Quantum Hall Effect, see [22, 14]). When there is no boundary, in dimension 2, the action of a perpendicular variable magnetic field (modeled by a 2D scalar vector field) modifies the transport properties of an electron gas ([35] for a physical approach). The most studied case is the so called *Iwatsuka model* corresponding to a magnetic field $\mathbf{B}(x, y) = \mathbf{B}(x)$ translationally invariant and x-increasing ([29]), tending to finite limits. The transport properties in the y direction are linked to the study of the *band functions*, that are the Fourier multipliers associated with the Hamiltonian (see [32, 17]). The particular case of a piecewise constant magnetic field acting on a 2D electron gas is considered in [42], and more mathematical properties associated with this model are described in [27, 16].

An analog model consists of a 3D planar translationally invariant magnetic field. Let us denote by (r, θ, z) the cylindrical coordinates of $\mathbb{R}^3$. We consider the magnetic potential $\mathbf{A}(r, \theta, z) = (0, 0, a(r))$ with $a(r)$ a suitable real function. The associated magnetic field is planar and is given by $\mathbf{B}(r, \theta, z) = b(r)(-\sin\theta, \cos\theta, 0)$ with $b(r) = a'(r)$. It is z-invariant and its field lines are circles contained in plans $\{z = z_0\}$ and centered at the origin of these plans. Under general assumptions on the function b, the classical trajectories of a particle in such a magnetic field are described in [44, Section 4]. The specific case of a magnetic field

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created by an infinite rectilinear current in the z direction is studied in [44, 10]: in that case $b(r) = r^{-1}$. The spectrum of $H_{\mathbf{A}}$ is the half-line $\mathbb{R}_+$ and the band functions are decreasing from $+\infty$ to 0. In [45] and [41], more general magnetic Hamiltonians with axisymmetric potentials are considered. The important particular case of a unitary magnetic field $b(r) = 1$ is treated in [45, Section 4]. The author shows that the band functions associated with axisymmetric functions of $\mathbb{R}^3$ loose their monotonicities and he deduces that the bottom of the spectrum of $H_{\mathbf{A}}$ is positive. In this note we study in more details the structure of the spectrum of the magnetic Hamiltonian for the case $b(r) = 1$ and we described the quantum states moving in such a magnetic field depending on their energy. We also make a natural comparison with an analog Hamiltonian in dimension 2, see below. Moreover, we explain how the operator studied here is linked to the magnetic Laplacian on wedges, a model appearing when studying the (Neumann) Schrödinger operator with large magnetic field in a domain with singular boundary (edges), see Section 1.3.

1.2. **Description of the Hamiltonians and problematic.** In this article we consider the magnetic potential defined in cartesian coordinates by $\mathcal{A}(x,y,z) := (0,0,\sqrt{x^2+y^2})$. The associated magnetic field $\mathcal{B} := \operatorname{curl}\mathcal{A}$ satisfies $\mathcal{B}(x,y,z) = (\sin\theta, -\cos\theta, 0)$ (where θ is the angular cylindrical coordinates of $\mathbb{R}^3$) and is unitary. Let

$$H_{\mathcal{A}} := (-i\nabla - \mathcal{A})^2 = D_x^2 + D_y^2 + (D_z - \sqrt{x^2+y^2})^2 \tag{1.1}$$

be the Hamiltonian associated with the magnetic field $\mathcal{B}$ acting on $L^2(\mathbb{R}^3)$. For an operator H, we denote by $\mathfrak{S}(H)$ its spectrum. Let

$$\Xi_0 := \inf \mathfrak{S}\left(H_{\mathcal{A}}\right) \tag{1.2}$$

be the ground state energy of $H_{\mathcal{A}}$. We know from [45] that $\mathfrak{S}(H_{\mathcal{A}}) = [\Xi_0, +\infty)$. Let $\mathcal{F}_z$ be the partial Fourier transform in the z-variable. We have the direct integral decomposition:

$$\mathcal{F}_z^* H_{\mathcal{A}} \mathcal{F}_z = \int_{\tau\in\mathbb{R}}^{\oplus} \boldsymbol{\ell}(\tau)\,\mathrm{d}\tau \tag{1.3}$$

with

$$\boldsymbol{\ell}(\tau) := -\Delta_{x,y} + (\|(x,y)\| - \tau)^2, \quad (x,y)\in\mathbb{R}^2 \tag{1.4}$$

where $\|\cdot\|$ denotes the euclidean norm of $\mathbb{R}^2$. The operator $\boldsymbol{\ell}(\tau)$ has compact resolvent and we denote by $\zeta_1(\tau)$ its first eigenvalue. Using (1.3) we have the fundamental relation

$$\Xi_0 = \inf_{\tau\in\mathbb{R}} \zeta_1(\tau)\ .$$

• *Study of the band functions and applications.* The study of $\boldsymbol{\ell}(\tau)$ reduces the problem to the singular 1D operators $\mathfrak{g}_m(\tau)$ (where $m \in \mathbb{Z}$ is the magnetic quantum number) introduced in Section 2.2. We denote by $(\zeta_{n,m}(\tau))_{n\in\mathbb{N}^*}$ its spectrum and we shorten the notation by $\zeta_{n,0} = \zeta_n$ when considering $m = 0$, which corresponds to restricting the operator to axisymmetric functions. The operator $H_{\mathcal{A}}$ is fibered and the functions $\tau \mapsto \zeta_{n,m}(\tau)$ are called the band functions (or dispersion curves). The study of their behavior is useful to describe many properties (transport and stability under perturbation) associated with $H_{\mathcal{A}}$. We are interested in the monotonicity properties and in the characterization of the infimum of $\zeta_1(\tau)$. As shown in [45], it is also remarkable that these band functions tend to finite limits when $\tau \to +\infty$ and are not contained in the general class of the band functions described in [20]. These limits are the Landau levels, that play the role of thresholds in the spectrum. The analysis of quantum states localized in energy far from the threshold is classical for fibered operators (see [32] for the Iwatsuka model and [20] for an abstract approach), but the situation needs a deeper analysis when looking at energies close to the thresholds. We will provide precise asymptotic expansion and describe the consequences on the properties (geometrical localization and current) of a quantum state localized in energy near a threshold in the spirit of the recent work [26].

• *The 2D analog model.* We recall here a standard analog 2D model. Let B_0 be the unitary translationally invariant magnetic field defined on $\mathbb{R}^2$ by $B_0(x,y) = \operatorname{sign}(x)$. Let $A_0(x,y) := (0, |x|)$ be a magnetic potential satisfying $\operatorname{curl} A_0 = B_0$. Notice the similar form with the vector fields $\mathcal{B}$ and $\mathcal{A}$ introduced above[1]. We denote by

$$H_0 := (-i\nabla - A_0)^2 = D_x^2 + (D_y - |x|)^2 \,, \quad (x,y) \in \mathbb{R}^2 \tag{1.5}$$

the associated Hamiltonian with $D = -i\partial$. In [42] the formal spectral analysis of the Hamiltonian H_0 allows to describe the transport properties of a 2D electron gas submitted to the magnetic field B_0. Formal arguments show that the quantum trajectories correspond to the classical one, the so-called *snake orbits*. Mathematical properties of the Hamiltonian H_0 for small electric perturbations are studied in [16] (see also [9] for a related Hamiltonian on a half-plane). Let $\Theta_0 := \inf \mathfrak{S}(H_0)$ be the bottom of the spectrum of the operator H_0. This spectral quantity has been introduced in [43] for a problem coming from the modeling of the phenomenon of "surface superconductivity" (see Section 1.3).

The study of the spectrum of H_0 leads to the 1D parameter family of operators

$$\mathfrak{h}_0(\tau) := -\partial_x^2 + (|x| - \tau)^2, \quad x \in \mathbb{R} \tag{1.6}$$

where $\tau \in \mathbb{R}$ is the Fourier variable dual to y. These well-known operators are sometimes known as the *de Gennes* operators (see Subsection 2.1 for references and former results). Once again, compare the above form with the operator $\boldsymbol{\ell}(\tau)$ defined in (1.4).

The operators $H_{\mathcal{A}}$ and $\boldsymbol{\ell}(\tau)$ studied in this article may be seen as versions of the operators H_0 and $\mathfrak{h}_0$ but in higher dimensions and one of our goals is to compare the associated band functions. It is known that the eigenvalues of $\mathfrak{h}_0(\tau)$ are exponentially close to the Landau levels for large τ. An application to the description of bulk states in one edge quantum system is given in [26]. Here, as we shall see, the band functions $\zeta_{n,m}$ converge polynomially toward the Landau levels, giving rise to different localization phenomena for the quantum states localized in energy near the thresholds. We also are interested in comparing the ground state energies Θ_0 and Ξ_0. Although this is a natural question when looking at similar quantum systems, this is also motivated by the link with a model operator on wedges as described in the paragraph below.

1.3. **Connection with the Laplacian on a domain with edges in the large magnetic field limit.** The modeling of the superconductivity phenomenon leads to study the minimizers of

[1] we may notice that the magnetic field B_0 corresponds to the profile of the magnetic field $\mathcal{B}(x,y,z)$ restricted to a plane $\{y = ax\}$

the Ginzburg-Landau functional. When applying a strong external magnetic field, the superconductivity phenomenon is destroyed. The linearization of the Ginzburg-Landau functional in that case leads to study the magnetic Laplacian with natural Neumann boundary conditions (see [21]). This operator is denoted by $H(\mathbf{A}, \Omega)$ where $\mathbf{A}$ is the magnetic potential and $\Omega \subset \mathbb{R}^3$ is the domain. The bottom of its spectrum is denoted by $\lambda(\mathbf{B}, \Omega)$. The critical value of the magnetic field for which the surface superconductivity appears in a type II superconductor Ω can be linked to $\lambda(\mathbf{B}, \Omega)$ (see [18] for more references). This gives an important motivation for the comprehension of the behavior of $\lambda(\mathbf{B}, \Omega)$ for large values of $\mathbf{B}$. For $x \in \overline{\Omega}$ we denote by Π_x the tangent cone to Ω at the point x and $\mathbf{B}_x := \mathbf{B}(x)$ the magnetic field frozen at x. A general fact is that $\lambda(\mathbf{B}, \Omega)$ behaves like $\inf_{x \in \overline{\Omega}} \lambda(\mathbf{B}_x, \Pi_x)$ for large magnetic fields. This is well-known for several specific cases (regular domains, 2D polygonal domains, cuboid), see [18] for an overview, and has been proved recently for general 3D corner domains ([7]). When the minimizers of $x \mapsto \lambda(\mathbf{B}_x, \Pi_x)$ are on the boundary of Ω, by studying the associated eigenvectors and coming back to the related non-linear Ginzburg-Landau problem, one expects surface superconductivity to appear for magnetic strength near the critical field (see [18]).

It is therefore crucial to have comparisons between all the possible values of $\lambda(\mathbf{B}_x, \Pi_x)$ for $x \in \overline{\Omega}$. When the boundary of Ω is regular, the tangent cones Π_x are either spaces or half-spaces. In this situation, the spectral model quantity $\lambda(\mathbf{B}_x, \Pi_x)$ is minimal and equal to Θ_0 (defined as the bottom of the spectrum of H_0, see above) when Π_x is a half-space with the magnetic field tangent to the boundary (see [31]). When the boundary of the domain has an edge of opening α, it is necessary to study the Neumann magnetic Laplacian on a new model domain: the infinite wedge of opening α denoted by $\mathcal{W}_\alpha$. First studies of this operator are presented in [34], [5] and [38] for case-specific geometries, and [37] for the general case. Let $\mathbf{B}$ be a constant magnetic field. We denote by $b_\perp$ the component of $\mathbf{B}$ orthogonal to the plane of symmetry of the wedge. If $b_\perp \neq 0$, the magnetic Laplacian $b_\perp^{-1} H(\mathbf{A}, \mathcal{W}_\alpha)$ degenerates formally toward the operator $H_{\mathcal{A}}$ when the opening angle α goes to 0, see [37, Lemma 5.1]. A formal analysis and several numerical computations show that $\lambda(\mathbf{B}, \mathcal{W}_\alpha)$ seems to converge to $b_\perp \Xi_0$ when the opening angle α goes to 0 (see [36, Chapter 6]). It is proved in [37, Section 5] that for all constant magnetic fields $\mathbf{B}$, there exists $C = C(\mathbf{B}) > 0$ such that

$$\forall \alpha \in (0, \pi], \quad \lambda(\mathbf{B}, \mathcal{W}_\alpha) \leqslant b_\perp \Xi_0 + C(\mathbf{B}) \alpha^2 .$$

Therefore the comparison between $b_\perp \Xi_0$ and the spectral model quantities associated with the points of the regular boundary of Ω (such as Θ_0) brings the asymptotics of the first eigenvalue of the magnetic Laplacian on a domain with an edge of small opening. In this article we provide an upper bound and numerical values for Ξ_0. We also prove $\Theta_0 < \Xi_0$. An application of the comparison between regular and singular model problems can be found in [39]. The semi-classical Laplacian with a constant magnetic field in a domain with a curved edge (a lens) is studied. The authors make an assumption on a 2D band function related to the conjecture 4.7 and use the tools of the semi-classical analysis to provide complete expansion of the eigenvalues of the magnetic Laplacian on the lens.

1.4. **Contents and main results.** In Section 2 we reduce the problem to a family of singular 1D Sturm-Liouville operators $(\mathfrak{g}_m(\tau))_{\tau\in\mathbb{R}}$ on the half-line and we recall basic properties of their eigenvalues $\zeta_{n,m}(\tau)$.

In section 3 we study these band functions when the Fourier parameter τ gets large, in particular we give in Proposition 3.4 a two-terms asymptotics

$$\zeta_{n,m}(\tau) = 2n - 1 + \frac{m^2 - \frac{1}{4}}{\tau^2} + O\left(\frac{1}{\tau^3}\right).$$

We then describe in Section 3.2 quantum states localized in energy near the thresholds: we show that there exist such states which are localized far from the z-axis and we provide an upper bound on their current by using the above asymptotics. This situation does not occur for quantum states localized in energy far from the thresholds.

In Section 4 we focus on $m = 0$ and we give an original formula for the derivative of $\zeta_n(\tau)$ with respect to τ. We then use it to prove that $\Theta_0 < \Xi_0$, showing that the ground state energy for these models is higher in dimension 3. We also give a criterion to characterize the minima of $\zeta_1(\tau)$. In Annex A we give numerical computations of $\zeta_1(\tau)$ and check that the criterion is numerically satisfied.

2. Description of the 1D operators

2.1. **The de Gennes operator.** We first recall known results about the fibers operator arising in the study of the Hamiltonian H_0 defined in (1.5). Let $\mathcal{F}_y$ be the partial Fourier transform in the y-variable. We have the following direct integral decomposition

$$\mathcal{F}_y^* H_0 \mathcal{F}_y := \int_{\tau\in\mathbb{R}}^{\oplus} \mathfrak{h}_0(\tau)\,\mathrm{d}\tau \tag{2.1}$$

where $\mathfrak{h}_0(\tau)$ is defined in (1.6). For all $\tau \in \mathbb{R}$ the operator $\mathfrak{h}_0(\tau)$ has compact resolvent and we denote by $\mu_n(\tau)$ its n-th eigenvalue. Let $\mathfrak{h}_0^{\mathrm{N}}(\tau)$ (resp. $\mathfrak{h}_0^{\mathrm{D}}(\tau)$) be the operator $\partial_x^2 + (x-\tau)^2$ acting on $L^2(\mathbb{R}_+)$ with Neumann (resp. Dirichlet) boundary condition in $x = 0$. We denote by $\mu_n^{\mathrm{N}}(\tau)$ (resp. $\mu_n^{\mathrm{D}}(\tau)$) its n-eigenvalue. Then for all $\mu_{2n-1}(\tau) = \mu_n^{\mathrm{N}}(\tau)$ and $\mu_{2n}(\tau) = \mu_n^{\mathrm{D}}(\tau)$ (see [18]). Moreover when τ goes to $+\infty$, both $\mu_{2n-1}(\tau)$ and $\mu_{2n}(\tau)$ converge toward the Landau level $2n-1$ (respectively by below and by above). The convergence is exponential, see [19] for a rough estimates and [26] for a precise asymptotic analysis.

Let $u_{n,\tau}$ be a normalized eigenfunction of $\mathfrak{h}_0^{\mathrm{N}}(\tau)$ associated with $\mu_n^{\mathrm{N}}(\tau)$. Using the techniques from [12] and [3], it is known that

$$(\mu_n^{\mathrm{N}})'(\tau) = (\tau^2 - \mu_n^{\mathrm{N}}(\tau))u_{n,\tau}^2(0) \tag{2.2}$$

and that there exists $\xi_0^n \in \mathbb{R}$ such that $\tau \mapsto \mu_n^{\mathrm{N}}(\tau)$ is decreasing on $(-\infty, \xi_0^n)$ and increasing on $(\xi_0^n, +\infty)$. Moreover the unique minimum of μ_n^{N} is non-degenerate and we have $\Theta_0 = \inf_\tau \mu_1^{\mathrm{N}}(\tau)$. If we denote by $\xi_0 := \xi_0^1$, (2.2) provides $\xi_0^2 = \Theta_0$. Using (2.1) we get $\inf \mathfrak{S}(H_0) = \Theta_0$. Numerical computations (see [43], [11] or [6] for a more rigorous analysis) show that $(\xi_0, \Theta_0) \approx (0.7682, 0.5901)$.

2.2. **Reduction to a 1D problem.** We reduce the study of the first eigenvalue of $\boldsymbol{\ell}(\tau)$ to a 1D singular Sturm-Liouville operator on a weighted space. In the polar coordinate (r,ϕ) the operator $\boldsymbol{\ell}(\tau)$ defined in (1.4) writes

$$-\partial_r^2-\frac{1}{r}\partial_r-\frac{1}{r^2}\partial_\phi^2+(r-\tau)^2\,,\quad (r,\phi)\in\mathbb{R}_+\times(-\pi,\pi)\,.$$

Let $L^2_r(\mathbb{R}_+)$ be the space of the functions squared integrable on the half axis $\mathbb{R}_+$ for the weight $r\,\mathrm{d}r$. We denote by

$$\langle u,v\rangle_{L^2_r(\mathbb{R}_+)}:=\int_{\mathbb{R}_+}u(r)v(r)r\,\mathrm{d}r$$

the scalar product associated with $L^2_r(\mathbb{R}_+)$. Let $B^1_r(\mathbb{R}_+):=\{u\in L^2_r,u'\in L^2_r(\mathbb{R}_+),ru\in L^2_r(\mathbb{R}_+)\}$. We define the operator

$$\mathfrak{g}_m(\tau)=-\partial_r^2-\frac{1}{r}\partial_r+\frac{m^2}{r^2}+(r-\tau)^2$$

on the domain

$$\begin{aligned}\mathrm{Dom}(\mathfrak{g}_m(\tau))=\{u\in B^1_r(\mathbb{R}_+),u''\in L^2_r(\mathbb{R}_+),\tfrac{1}{r}u'\in L^2_r(\mathbb{R}_+),\tfrac{1}{r^2}u\in L^2_r(\mathbb{R}_+),&\\ r^2u\in L^2_r(\mathbb{R}_+),(ru'(r))_{|r=0}=0\}\,.&\end{aligned}\tag{2.3}$$

The form domain of $\mathfrak{g}_m(\tau)$ is $\{u\in B^1_r(\mathbb{R}_+),\frac{1}{r}u\in L^2(\mathbb{R}_+)\}$ and the associated quadratic form is

$$\mathfrak{q}^\tau_m(u):=\int_{\mathbb{R}_+}\left(|u'(r)|^2+\frac{m^2}{r^2}|u(r)|^2+(r-\tau)^2|u(r)|^2\right)r\,\mathrm{d}r\,.$$

Using the results from [4] we get that the operator $\mathfrak{g}_m(\tau)$ has compact resolvent and we denote by $\zeta_{n,m}(\tau)$ its n-th eigenvalue and $z_{n,m}(\cdot,\tau)$ an associated eigenvector. We shorten the notation when $m=0$ by using $\zeta_{n,0}=\zeta_n$ and $z_n(\cdot,\tau)=z_{n,m}(\cdot,\tau)$. Then $\boldsymbol{\ell}(\tau)$ is unitarily equivalent to $\bigoplus_{m\in\mathbb{Z}}\mathfrak{g}_m(\tau)$ and therefore (see also (1.3)):

$$\Xi_0=\inf_{\tau\in\mathbb{R}}\zeta_1(\tau)\,,\tag{2.4}$$

moreover the $(\zeta_n(\tau))_{n\geqslant 0}$ are the eigenvalues of $\boldsymbol{\ell}(\tau)$ which have axisymmetric eigenfunctions.

2.3. **Elementary results about the spectrum of the 1D operator.** The boundary value problem associated with the eigenvalue $\zeta_n(\tau)$ is the following:

$$\begin{cases}-ru''(r)-u'(r)+r(r-\tau)^2u(r)=r\zeta_n(\tau)u(r)\,,\quad r>0\,, & \text{(2.5a)}\\ ru'(r)_{|r=0}=0\,. & \text{(2.5b)}\end{cases}$$

The differential equation (2.5a) is singular and the point $r=0$ is regular singular, therefore using Fuchs theory and the boundary condition (2.5b) we get (see [36, Proposition 6.4] for more details and [45, Lemma 4.1] for a more general case):

Proposition 2.1. *For all $\tau\in\mathbb{R}$ and for all $n\geqslant 1$, $\zeta_n(\tau)$ is a simple eigenvalue of $\mathfrak{g}_0(\tau)$. We denote by $z_n(\cdot,\tau)$ an associated eigenfunction. The function $z_n(\cdot,\tau)$ is the restriction on $\mathbb{R}_+$ of an analytic function on $\mathbb{R}$, moreover it satisfies the Neumann boundary condition*

$$z'_n(0,\tau)=0\,.\tag{2.6}$$

Since the form domain of $\mathfrak{g}_0(\tau)$ does not depend on τ, we deduce from Kato's theory (see [30]) that all the $\zeta_n(\tau)$ are analytic with respect to τ. Moreover the Feynman-Hellmann ([28]) formula provides

$$\forall n \geqslant 1, \forall \tau \in \mathbb{R}, \quad \zeta_n'(\tau) = -2\int_{\mathbb{R}_+} (r-\tau)^2 z_n(r,\tau) r \,\mathrm{d}r \,, \tag{2.7}$$

and we deduce that for all $n \geqslant 1$, the function $\tau \mapsto \zeta_n(\tau)$ is decreasing on $(-\infty, 0)$.

In the special case $\tau = 0$, the operator $\mathfrak{g}_m(0)$ is also known as the Laguerre operator (see [1]) whose eigenvalues are known:

$$\forall n \geqslant 1, \quad \zeta_{n,m}(0) = 4n - 2 + 2|m| \,.$$

Remark 2.2. The eigenvalues of the 2D harmonic oscillator $\boldsymbol{\ell}(0) = -\Delta + \|(x,y)\|^2$ with $(x,y) \in \mathbb{R}^2$ are the even positive integers. Only the eigenspaces associated with eigenvalues of the form $4n-2$ have axisymmetric eigenfunctions.

3. Asymptotic of the band functions and application to the description of quantum states

3.1. **Limits for large Fourier parameters.** Using the lower bound $(r-\tau)^2 \geqslant \tau^2$ for $\tau \leqslant 0$ we deduce from the min-max principle that for all $\tau \leqslant 0$ we have $\zeta_{n,m}(\tau) \geqslant \tau^2$ and therefore

$$\lim_{\tau \to -\infty} \zeta_{n,m}(\tau) = +\infty \,. \tag{3.1}$$

In the case of the de Gennes operator $\mathfrak{h}_0(\tau)$, the eigenfunctions concentrate for large τ in the well of the potential $(r-\tau)^2$ and therefore the eigenvalues of $\mathfrak{h}_0(\tau)$ converge toward the Landau levels for large τ (see Section 2.1). This is again true for the eigenvalues of the operator $\mathfrak{g}_m(\tau)$, indeed the potential satisfies the hypothesis of [45, Proposition 3.6] and we deduce:

$$\forall (n,m) \in \mathbb{N}^* \times \mathbb{Z}, \quad \lim_{\tau \to +\infty} \zeta_{n,m}(\tau) = 2n-1 \,. \tag{3.2}$$

However we work in a weighted space and the harmonic approximation that consists in using the Hermite's functions as quasi-modes is not as good as in the case of the de Gennes operator. It is proven in [45, Proposition 4.7] that

$$\forall n \geqslant 1, \quad \exists \gamma_n > 0, \exists \tau_n > 0, \forall \tau > \tau_n, \quad \zeta_n(\tau) \leqslant (2n-1) - \gamma_n \tau^{-2} \,. \tag{3.3}$$

We give a two-terms asymptotics of all the band functions $\zeta_{n,m}$ for large τ:

Proposition 3.1. *For all $(n,m) \in \mathbb{N}^* \times \mathbb{Z}$ we have*

$$\zeta_{n,m}(\tau) \underset{\tau \to +\infty}{=} 2n - 1 + \frac{m^2 - \frac{1}{4}}{\tau^2} + O\left(\frac{1}{\tau^3}\right) \,. \tag{3.4}$$

In particular, only the eigenvalues associated with axisymmetrical eigenfunctions ($m = 0$) are below their limit.

Proof. We define the unitary transform $\mathcal{M} : u(r) \mapsto \sqrt{r}\, u(r)$ from $L^2_r(\mathbb{R}_+)$ into $L^2(\mathbb{R}_+)$. Then $\mathcal{M}\mathfrak{g}_m(\tau)\mathcal{M}^*$ expressed as

$$-\partial_r^2 + \frac{m^2 - \frac{1}{4}}{r^2} + (r-\tau)^2 \, , r > 0$$

acting now on the unweighted space $L^2(\mathbb{R}_+)$. Using now the change of variable $x = r - \tau$, we are led to study

$$\widetilde{\mathfrak{g}}_m(\tau) := -\partial_x^2 + \tau^{-2}\frac{m^2 - \frac{1}{4}}{(1+\tau^{-1}x)^2} + x^2, \quad x > -\tau \, .$$

The remain of the proof is now standard and is based on the harmonic approximation procedure ([15, Chapter 4]), at the difference that our functions are not defined on the entire real axis but only on $(-\tau, +\infty)$. A very similar situation is described with full details in [10, Section 2] and we give below elements of proof. We write

$$\widetilde{\mathfrak{g}}_m(\tau) = \mathfrak{h}^\infty + \tau^{-2}(m^2 - \tfrac{1}{4}) + V_\tau$$

where $\mathfrak{h}^\infty := -\partial_x^2 + x^2$ is the harmonic oscillator and V_τ is controlled near the well $\{x = 0\}$:

$$\exists x_0 > 0, \exists C > 0, \; \forall x \in (-x_0, x_0), \; \forall \tau \geqslant 1, \quad |V_\tau(x)| \leqslant C\frac{|x|}{\tau^3} \, . \tag{3.5}$$

We apply a cut-off to the Hermite's functions (that are the eigenfunctions of $\mathfrak{h}^\infty$ associated with the Landau levels $2n-1$) and we use the resulting functions as quasi-modes for the operator $\widetilde{\mathfrak{g}}_m(\tau)$. The min-max principle combined with (3.5) provides the upper bound of (3.4). The lower bound relies on Agmon estimates showing that the eigenfunctions of $\widetilde{\mathfrak{g}}_m(\tau)$ are concentrated in the well of the potential $\{x = 0\}$ when $\tau \to +\infty$. A standard procedure consists then in using the (truncated) eigenfunctions of $\widetilde{\mathfrak{g}}_m(\tau)$ as quasi-modes for $\mathfrak{h}^\infty$, as in [23, Chapter 3]). Using that the eigenvalues $\zeta_{n,m}(\tau)$ are well separated for different n and large τ (see (3.2)) we conclude to the lower bound of (3.4) by using the spectral theorem. □

Remark 3.2. It is possible to reach a full asymptotic expansion of $\zeta_{n,m}(\tau)$ in power of τ^{-1} for large τ by using a series expansion of the potential V_τ.

Remark 3.3. It is also possible to add an electric perturbation to the magnetic Hamiltonians H_0 and $H_{\mathcal{A}}$. The associated Krein spectral shift function (see [2] for an overview on the spectral shift function) will have singularities near the Landau levels $2n-1$ who play the role of thresholds in the spectrum of the operators H_0 and $H_{\mathcal{A}}$. The asymptotic behavior of the spectral shift function near the thresholds depends among other things on the behavior of the band functions at energies close to the thresholds (see for example [8] for a study of a magnetic Hamiltonian on a half-strip). Since the band functions $\mu_n(\tau)$ and $\zeta_{n,m}(\tau)$ have different behaviors for large τ, we expect that the spectral shift function associated with perturbations of the Hamiltonians H_0 and $H_{\mathcal{A}}$ will have different singular behaviors when approaching the Landau levels.

3.2. **Description of quantum states localized in energy near the thresholds.** In this section we describe briefly how the previous asymptotics can be used to describe quantum states localized in energy near the thresholds in the spirit of the approach developed in [26]. For simplicity we focus on $m = 0$, which corresponds to axisymmetric states. Our analysis extends easily to the case $m \neq 0$. For such a state $\psi \in L^2(\mathbb{R}^3)$ we denote by $\psi_n(\tau) := \langle \mathcal{F}_z\psi(\cdot,\tau), z_n(\cdot,\tau)\rangle_{L^2_r(\mathbb{R}_+)}$ its n-th Fourier coefficient. There holds the following decomposition:

$$\psi(r,z) = \sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}} e^{i\tau z}\psi_n(\tau)z_n(r,\tau)\,\mathrm{d}\tau \quad \text{and} \quad \sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}} |\psi_n(\tau)|^2\,\mathrm{d}\tau = \|\psi\|^2_{L^2(\mathbb{R}^3)}\,. \tag{3.6}$$

For a bounded interval $I \subset \mathfrak{S}(H_{\mathcal{A}})$, we denote by $\mathbb{P}_I$ the spectral projection on I associated with $H_{\mathcal{A}}$. We describe here the properties of a quantum state ψ localized in energy in I, that is a function $\psi \in L^2(\mathbb{R}^3)$ satisfying $\mathbb{P}_I\psi = \psi$. In that case all the Fourier coefficient $\tau \mapsto \psi_n(\tau)$ are supported into $\zeta_n^{-1}(I)$.

Recall that the Landau levels $2n-1$ are the thresholds of H_0 as the limits of the $\zeta_n(\tau)$ for large τ. Therefore when I does not contain any threshold, $\zeta_n^{-1}(I)$ is a finite reunion of bounded intervals and the analysis from De Bièvre and Pulé ([14]) shows that such a quantum state is geometrically localized near the z-axis.

Conversely, we expect that a quantum states localized in energy near a Landau level may be localized far from the z-axis. This is indeed the case: set $n \in \mathbb{N}^*$, let $\delta > 0$ be a small energy parameter and consider $I_\delta := (2n-1-\delta, 2n-1+\delta)$. When $n' \neq n$, due to (3.1), the set $\zeta_{n'}^{-1}(I_\delta)$ is still bounded. However due to the continuity of ζ_n, we have $\zeta_n^{-1}(I_\delta) = J_\delta \cup (\tau_n(\delta), +\infty)$ where J_δ is a bounded set. Moreover due to (3.4) we have

$$\tau_n(\delta) \underset{\delta\to 0}{\sim} \sqrt{\frac{1}{4\delta}}\,. \tag{3.7}$$

Assume that ψ is localized in energy in I_δ. When $\mathrm{Supp}(\psi_n) \subset J_\delta$, ψ is geometrically localized near the z-axis. Assume now that $\mathrm{Supp}(\psi_n) \subset (\tau_n(\delta), +\infty)$. Due to standard Agmon estimates, the eigenfunctions $r \mapsto z_n(r,\tau)$ associated with $\zeta_n(\tau)$ are localized near the well of the potential $\{r = \tau\}$ when τ gets large. Therefore as in [26, Section 4], one can show by using (3.6) and (3.7) that ψ is localized at a distance at least $O(\delta^{-1/2})$ from the z-axis when δ gets small, showing that such a state is localized far from the variations of the magnetic field $\mathcal{B}$.

We now show that the states described above do not propagate along the z-axis, as expected of the classical picture. We define the current operator as the commutator $[H_{\mathcal{A}}, z]$. It is well-known that the spectrum of this observable can be interpreted as the velocity along the z-axis of a quantum state moving in the magnetic field $\mathcal{B}$. Standard computations (see [14], [32]) based on (3.6) and Feynman-Hellmann formula show that for all quantum states ψ localized in energy in I and such that $\mathrm{Supp}(\psi_n) \subset (\tau_n(\delta), +\infty)$ there holds

$$|\langle [H_{\mathcal{A}}, z]\psi, \psi\rangle| \leqslant \sup_{\tau\in(\tau_n(\delta),+\infty)} |\zeta_n'(\tau)|\|\psi\|^2_{L^2(\mathbb{R}^3)}\,, \tag{3.8}$$

linking the current operator with the derivative of the band functions. Some tedious computations show that the asymptotics of $\zeta_n'(\tau)$ for large τ is directly derived from the one of $\zeta_n(\tau)$ (see [26, Section 3]) for a similar situation with full details). In particular, due to (3.7):

$$|\zeta_n'(\tau_n(\delta))| \underset{\delta\to 0}{\sim} 8\delta^{3/2}\,.$$

Using (3.8), we deduce that the current borne by quantum states localized in energy in I_δ and far from the z-axis is controlled by $O(\delta^{3/2})$ when δ gets small.

We summarize now the situation: given an interval $I \subset \mathfrak{S}(H_{\mathcal{A}})$ that contains a threshold, a quantum state ψ localized in I is the superposition of the following:

- A component localized near the z-axis, whose Fourier coefficients are compactly supported. This component may be called *edge state*.
- A component localized far from the z-axis and bearing a small current, whose Fourier coefficient are supported in an interval of the form $(\tau_n, +\infty)$. This component is typical of the presence of a threshold in I. By comparison with the physical literature, we may call this component *bulk state*.

Remark 3.4. Unlike to the band functions $\mu_n(\tau)$ associated with the operator H_0, the convergence of $\zeta_n(\tau)$ toward the Landau levels is not exponential. This is why the localization properties and the current borne by quantum state localized in energy near the thresholds are different from those described in [26].

4. Characterization of the minimum

4.1. **Rough upper bound for the ground state energy.** Using the estimation (3.3), it is proved in [45, Theorem 4.9] that all the functions $\tau \mapsto \zeta_n(\tau)$ loose their monotonicity for $\tau > 0$ and reach their infimum. We provide an upper bound for the infimum of $\tau \mapsto \zeta_1(\tau)$:

Proposition 4.1. *We have*

$$\Xi_0 \leqslant \sqrt{4-\pi} \tag{4.1}$$

and there exists $\tau^* \in \mathbb{R}$ such that $\Xi_0 = \zeta_1(\tau^*)$.

Proof. In order to get an upper bound we use gaussian quasi-modes: for $\gamma > 0$ we define $u_\gamma(r) := e^{-\gamma r^2}$. Computations yield:

$$\frac{\mathfrak{q}_0^\tau(u_\gamma)}{\|u_\gamma\|^2_{L^2_r(\mathbb{R}_+)}} = 2\gamma + \frac{1}{2\gamma} + \tau^2 - \tau\left(\frac{\pi}{2\gamma}\right)^{1/2} .$$

We minimize the right hand side by choosing $\gamma = \frac{\pi}{8\tau^2}$ and we deduce from the min-max principle:

$$\zeta_1(\tau) \leqslant \frac{\pi}{4}\frac{1}{\tau^2} + \frac{4-\pi}{\pi}\tau^2 .$$

This upper bound is minimal for $\tau = (\frac{\pi^2}{4(4-\pi)})^{1/4}$ and provides (4.1) by using (2.4). $\square$

4.2. **Comparison between the lowest energies.** In this section we focus on the case $m = 0$. We give a new expression of the derivative of the function ζ_n. We use it to get a comparison between Θ_0 and Ξ_0.

In order to have a parameter-independent potential, we perform the translation $\rho = r - \tau$ and we get that $\mathfrak{g}_0(\tau)$ is unitarily equivalent to the operator

$$\hat{\mathfrak{g}}_0(\tau) := -\partial_\rho^2 - \frac{1}{\rho+\tau}\partial_\rho + \rho^2 , \quad \rho > -\tau$$

acting on $L^2_{\rho+\tau}(I_\tau)$ with $I_\tau := (-\tau, +\infty)$. The domain of the operator $\hat{\mathfrak{g}}_0(\tau)$ is deduced from $\mathrm{Dom}(\mathfrak{g}_0(\tau))$ using the translation $\rho = r - \tau$. The interval I_τ depends now on the parameter. Usually the techniques from [12] and [13] give a trace formula for the derivative with respect to the boundary of the eigenvalues of such an operator (see the formula (2.2) for example). However the results of [13] specific to weighted spaces cannot be applied, indeed the weight $\rho + \tau$ depends on the parameter τ. We prove à la "Bolley-Dauge-Helffer" a formula for the derivative that is of a different kind from (2.2) and [13, Theorem 1.8]. To our knowledge this formula is independent from the Feynman-Hellmann formula (2.7):

Proposition 4.2. *Let $n \geqslant 1$ and let $z_n(\cdot,\tau)$ be a normalized eigenfunction associated with $\zeta_n(\tau)$ for the operator $\mathfrak{g}_0(\tau)$. We have*

$$\zeta_n'(\tau) = \langle (\mathfrak{h}_0^{\mathrm{N}}(\tau) - \zeta_n(\tau)) z_n(\cdot,\tau), z_n(\cdot,\tau)\rangle_{L^2(\mathbb{R}_+)} \ . \tag{4.2}$$

Proof. We denote by $\hat{z}_n(\rho,\tau) := z_n(\rho+\tau,\tau)$ a normalized eigenfunction of $\hat{\mathfrak{g}}_0(\tau)$ associated with $\zeta_n(\tau)$. It satisfies

$$-\hat{z}_n''(\rho,\tau) - \frac{\hat{z}_n'(\rho,\tau)}{\rho+\tau} + \rho^2 \hat{z}_n(\rho,\tau) = \zeta_n(\tau)\hat{z}_n(\rho,\tau) \ . \tag{4.3}$$

For $h > 0$ we introduce the quantity

$$d_{n,\tau}(h) := (\zeta_n(\tau+h) - \zeta_n(\tau)) \langle \hat{z}_n(\cdot,\tau+h), \hat{z}_n(\cdot,\tau)\rangle_{L^2_{\rho+\tau}(I_\tau)} \ .$$

The analyticity of the eigenpairs $(\zeta_n(\tau), \hat{z}_n(\cdot,\tau))_{n\in\mathbb{N}}$ is a direct consequence of the simplicity of the eigenvalues (see proposition 2.1) and of Kato's theory. Since the $\hat{z}_n(\cdot,\tau)$ are normalized in $L^2_{\rho+\tau}(I_\tau)$ we deduce that

$$\lim_{h\to 0} \frac{d_{n,\tau}(h)}{h} = \zeta_n'(\tau) \ . \tag{4.4}$$

On the other side using the eigenvalue equation (4.3) we get:

$$\begin{aligned}
d_{n,\tau}(h) &= \int_{-\tau}^{+\infty} \big(\zeta_n(\tau+h)\hat{z}_n(\rho,\tau+h)\hat{z}_n(\rho,\tau) - \zeta_n(\tau)\hat{z}_n(\rho,\tau+h)\hat{z}_n(\rho,\tau)\big)(\rho+\tau)\,\mathrm{d}\rho \\
&= \int_{-\tau}^{+\infty} \left(-\hat{z}_{n,\tau+h}''(\rho) - \frac{1}{\rho+\tau+h}\hat{z}_n'(\rho,\tau+h) + \rho^2\hat{z}_n(\rho,\tau+h)\right) \hat{z}_n(\rho,\tau)(\rho+\tau)\,\mathrm{d}\rho \\
&\quad - \int_{-\tau}^{+\infty} \left(-\hat{z}_\tau''(\rho) - \frac{1}{\rho+\tau}\hat{z}_n'(\rho,\tau) + \rho^2\hat{z}_n(\rho,\tau)\right) \hat{z}_n(\rho,\tau+h)(\rho+\tau)\,\mathrm{d}\rho \ .
\end{aligned}$$

We make integrations by parts on the terms with second derivative:

$$\begin{aligned}
d_\tau(h) &= \int_{-\tau}^{+\infty} \hat{z}_n'(\rho,\tau+h)\big((\rho+\tau)\hat{z}_n'(\rho,\tau) + \hat{z}_n(\rho,\tau)\big) - \frac{\rho+\tau}{\rho+\tau+h}\hat{z}_n'(\rho,\tau+h)\hat{z}_n(\rho,\tau)\,\mathrm{d}\rho \\
&\quad + \int_{-\tau}^{+\infty} -\hat{z}_n'(\rho,\tau)\big((\rho+\tau)\hat{z}_n'(\rho,\tau+h) + \hat{z}_n(\rho,\tau+h)\big) + \hat{z}_n'(\rho,\tau)\hat{z}_n(\rho,\tau+h)\,\mathrm{d}\rho \\
&= h\int_{-\tau}^{+\infty} \frac{1}{\rho+\tau+h}\hat{z}_n'(\rho,\tau+h)\hat{z}_n(\rho,\tau)\,\mathrm{d}\rho \ .
\end{aligned}$$

Thanks to (4.4) and to the analyticity of the eigenpairs with respect to the parameter we have
$$\zeta_n'(\tau) = \int_{-\tau}^{+\infty} \frac{1}{\rho+\tau} \hat{z}_n'(\rho,\tau)\hat{z}_n(\rho,\tau)\,\mathrm{d}\rho\,.$$
Using (4.3) we deduce
$$\zeta_n'(\tau) = \int_{-\tau}^{+\infty} \left(-\hat{z}_n''(\rho,\tau) + \rho^2\hat{z}_n(\rho,\tau) - \zeta_n(\tau)\hat{z}_n(\rho,\tau)\right)\hat{z}_n(\rho,\tau)\,\mathrm{d}\rho\,.$$
We make the translation $\rho = r-\tau$:
$$\zeta_n'(\tau) = \int_{\mathbb{R}_+} \left(-\hat{z}_n''(r,\tau) + \left((r-\tau)^2 z_n(r,\tau) - \zeta_n(\tau)z_n(r,\tau)\right)\right) z_n(r,\tau)\,\mathrm{d}r\,.$$
Thanks to (2.6), we have $z_n(\cdot,\tau) \in \mathrm{Dom}(\mathfrak{h}_0^{\mathrm{N}}(\tau))$ and we deduce (4.2). □

This formula is not sufficient to give direct informations on the monotonicity of the functions $\tau \mapsto \zeta_n(\tau)$. However it provides the following comparison between the bottom of the spectrum of the 2D Hamiltonian H_0 and the one of the 3D Hamiltonian $H_{\mathcal{A}}$:

Theorem 4.3. *We have*
$$\Theta_0 < \Xi_0\,.$$

Proof. Let τ^* be a point such that $\zeta_1(\tau^*) = \Xi_0$ (see Proposition 4.1). We have $\zeta_1'(\tau^*) = 0$ and thanks to Proposition 4.2:
$$\zeta_1(\tau^*) = \frac{\langle \mathfrak{h}_0^{\mathrm{N}}(\tau^*)z_1(\cdot,\tau^*), z_1(\cdot,\tau^*)\rangle_{L^2(\mathbb{R}_+)}}{\|z_1(\cdot,\tau^*)\|^2_{L^2}(\mathbb{R}_+)}\,.$$
We deduce from the min-max principle that $\zeta_1(\tau^*) \geqslant \mu_1^{\mathrm{N}}(\tau^*)$. Let us suppose that we have the equality $\zeta_1(\tau^*) = \mu_1^{\mathrm{N}}(\tau^*)$, then $z_1(\cdot,\tau^*)$ is a minimizer of the quadratic form associated with $\mathfrak{h}_0^{\mathrm{N}}(\tau^*)$ and since $z_1(\cdot,\tau^*)$ satisfies the Neumann boundary condition (2.6), it is an eigenfunction of $\mathfrak{h}_0^{\mathrm{N}}(\tau^*)$ associated with $\mu_1^{\mathrm{N}}(\tau^*)$:
$$\forall r>0, \quad -z_1''(r,\tau^*) + (r-\tau^*)^2 z_1(r,\tau^*) = \mu_1^{\mathrm{N}}(\tau^*)z_1(r,\tau^*)\,.$$
Combining this with (2.5a) we get $z_1'(\cdot,\tau^*) = 0$ on $\mathbb{R}_+$, which is absurd. Therefore we have $\Xi_0 = \zeta_1(\tau^*) > \mu_1^{\mathrm{N}}(\tau^*) \geqslant \Theta_0$. □

4.3. **A criterion for the characterization of the minimum.** In [45, Section 4], the author adresses the question of knowing how many minima has the band function $\tau \mapsto \zeta_n(\tau)$. We give here a criterion in order to characterize the critical points of ζ_1. Numerical simulations show that this criterion seems to be satisfied. Let us notice that most of the techniques presented here can be found in [25] and [24]. In the following we denote by $z_1(\cdot,\tau)$ a normalized eigenfunction of $\mathfrak{g}_0(\tau)$ associated with $\zeta_1(\tau)$. Since $\zeta_1(\tau)$ is simple, $\tau \mapsto z_1(\cdot,\tau)$ is analytic and we denote by $\dot{z}_1(r,\tau) := \partial_\tau z(r,\tau)$.

Lemma 4.4. *We have*
$$\forall \tau \in \mathbb{R}, \quad \|\dot{z}_1(\cdot,\tau)\|_{L^2_r(\mathbb{R}_+)} \leqslant \frac{2}{\zeta_2(\tau)-\zeta_1(\tau)}\|(r-\tau)z_1(\cdot,\tau)\|_{L^2_r(\mathbb{R}_+)}\,.$$

Proof. We differentiate $\|z_1(\cdot,\tau)\|^2_{L^2_r(\mathbb{R}_+)} = 1$ with respect to τ and we get that $\dot{z}_1(\cdot,\tau)$ is orthogonal to $z_1(\cdot,\tau)$ in $L^2_r(\mathbb{R}_+)$. We deduce from the min-max principle:

$$(\zeta_2(\tau)-\zeta_1(\tau))\|\dot{z}_1(\cdot,\tau)\|^2_{L^2_r(\mathbb{R}_+)} \leqslant \langle(\mathfrak{g}_0(\tau)-\zeta_1(\tau))\dot{z}_1(\cdot,\tau),\dot{z}_1(\cdot,\tau)\rangle_{L^2_r(\mathbb{R}_+)}.$$

We differentiate $\mathfrak{g}_0(\tau)z_1(\cdot,\tau)=\zeta_1(\tau)z_1(\cdot,\tau)$ with respect to τ and we get $(\mathfrak{g}_0(\tau)-\zeta_1(\tau))\dot{z}_1(\cdot,\tau) = -\partial_\tau\mathfrak{g}_0(\tau)z_1(\cdot,\tau)$, therefore

$$(\zeta_2(\tau)-\zeta_1(\tau))\|\dot{z}_1(\cdot,\tau)\|^2_{L^2_r(\mathbb{R}_+)} \leqslant \langle -\partial_\tau\mathfrak{g}_0(\tau)z_1(\cdot,\tau),\dot{z}_1(\cdot,\tau)\rangle_{L^2_r(\mathbb{R}_+)} .$$

By using Cauchy-Schwarz inequality and the identity $\partial_\tau\mathfrak{g}_0(\tau) = -2(r-\tau)$ we deduce the Lemma. ☐

Lemma 4.5 (Virial identity)**.** *Let τ_{C} be a critical point of ζ_1. Then we have*

$$\int_{\mathbb{R}_+} r|z_1'(r,\tau_{\mathrm{C}})|^2\,\mathrm{d}r = \int_{\mathbb{R}_+}(r-\tau_{\mathrm{C}})^2|z_1(r,\tau_{\mathrm{C}})|^2 r\,\mathrm{d}r = \frac{\zeta_1(\tau_{\mathrm{C}})}{2}\,. \tag{4.5}$$

Proof. We introduce the scaled operator

$$\mathfrak{g}_0(\tau,a) := -a^{-2}\frac{1}{r}\partial_r r\partial_r + (ar-\tau)^2,\quad a>0$$

which is unitarily equivalent to $\mathfrak{g}_0(\tau)$. We denote by $z^a(r,\tau) := z_1(\frac{r}{a},\tau)$ and we have

$$\forall a>0,\quad (\mathfrak{g}_0(\tau,a)-\zeta_1(\tau))\,z^a(\cdot,\tau) = 0\,.$$

We differentiate this relation with respect to a:

$$(\mathfrak{g}_0(\tau,a)-\zeta_1(\tau))\,\partial_a z^a(\cdot,\tau) + \partial_a\mathfrak{g}_0(\tau,a)z^a(\cdot,\tau) = 0 \tag{4.6}$$

with

$$\partial_a\mathfrak{g}_0(\tau,a) = 2a^{-3}\frac{1}{r}\partial_r r\partial_r + 2r(ar-\tau)\,.$$

We make the scalar product of (4.6) with $z^a(\cdot,\tau)$ in $L^2_r(\mathbb{R}_+)$ and we take $a=1$:

$$\int_{\mathbb{R}_+}\left(-2|z_1'(r,\tau)|^2 + 2r(r-\tau)|z_1(r,\tau)|^2\right) r\,\mathrm{d}r = 0\,. \tag{4.7}$$

Thanks to (2.7), if τ_{C} is a critical point of ζ_1 we have

$$\int_{\mathbb{R}_+}(r-\tau_{\mathrm{C}})|z_1(r,\tau_{\mathrm{C}})|^2 r\,\mathrm{d}r = 0$$

and therefore

$$\int_{\mathbb{R}_+}(r-\tau_{\mathrm{C}})^2|z_1(r,\tau_{\mathrm{C}})|^2 r\,\mathrm{d}r = \int_{\mathbb{R}_+} r(r-\tau_{\mathrm{C}})|z_1(r,\tau_{\mathrm{C}})|^2 r\,\mathrm{d}r\,. \tag{4.8}$$

Since

$$\forall\tau\in\mathbb{R},\quad \int_{\mathbb{R}_+}\left(|z_1'(r,\tau)|^2 + (r-\tau)^2|z_1(r,\tau)|^2\right) r\,\mathrm{d}r = \zeta_1(\tau),$$

by using (4.7) and (4.8) we get (4.5). ☐

We can now state our criterion: if the spectral gap is large enough in a critical point of ζ_1, this critical point is a non-degenerate minimum:

Proposition 4.6. *Let τ_{C} be a critical point of ζ_1. Then we have*

$$\zeta_1''(\tau_{\mathrm{C}}) \geqslant 2\frac{\zeta_2(\tau_{\mathrm{C}})-3\zeta_1(\tau_{\mathrm{C}})}{\zeta_2(\tau_{\mathrm{C}})-\zeta_1(\tau_{\mathrm{C}})}\,. \tag{4.9}$$

Proof. We first differentiate the Feynman-Hellmann relation (2.7) and we get

$$\forall \tau \in \mathbb{R}, \quad \zeta_1''(\tau) = 2 - 4\int_{\mathbb{R}_+}(r-\tau)\dot{z}_1(r,\tau)z_1(r,\tau)r\,\mathrm{d}r\,.$$

The Cauchy-Schwarz inequality and the Lemma 4.4 provide

$$\zeta_1''(\tau) \geqslant 2 - \frac{8\|(r-\tau)z_1(\cdot,\tau)\|^2_{L^2_r(\mathbb{R}_+)}}{\zeta_2(\tau)-\zeta_1(\tau)}\,.$$

If τ_{C} is a critical point of ζ_1, we deduce (4.9) from the Lemma 4.5. □

We know that $\zeta_2(0)-3\zeta_1(0) = 0$ and that $\zeta_2 - 3\zeta_1$ goes to 0 for τ large (see Proposition 3.2). Moreover numerical simulations show that $\zeta_2 - 3\zeta_1$ seems to be positive on $(0,+\infty)$, see figure 2. We already know that ζ_1 is non-increasing on $(-\infty, 0)$, therefore using Proposition 4.6 we believe that all the critical points of ζ_1 are minima. Therefore we are led to make the following:

Conjecture 4.7. *The band function $\tau \mapsto \zeta_1(\tau)$ has a unique and non-degenerate minimum.*

Remark 4.8. Let us notice that similar conjectures can be found in the literature: in [39], the characterization of the minimum of the band function of a related model problem would bring localization property for the semi-classical Laplacian of a domain with a curved edge. In [44] the author makes a conjecture on the monotonicity of the derivative of a band function associated with a magnetic Hamiltonian in $\mathbb{R}^3$. Using the techniques from [44, Section 3] and [45, Section 5], the conjecture 4.7 can bring scattering properties for the Hamiltonian $H_{\mathcal{A}}$. Moreover if the conjecture 4.7 is true, we will be able to describe the number of eigenstates created under the action of a suitable electric perturbation (see [40]).

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Appendix A. Numerical approximations

The numerical approximations described here use the finite element library Mélina ([33]). We refer to [36, Subsection 6.2.4] for more simulations and computation details. We denote by $\breve{\zeta}_n(\tau)$ a numerical approximation of $\zeta_n(\tau)$. The figure 1 presents the numerical approximations $\breve{\zeta}_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \leqslant k \leqslant 500$. The numerical approximations have a unique minimum $\breve{\Xi}_0 = 0.8630$ and the corresponding minimizing Fourier parameter is $\breve{\tau}^* = 1.53$. We also plot the constant $\Theta_0 \approx 0.5901$ according to the computation of [6] and the upper bound $\sqrt{4-\pi} \approx 0.9265$ given by Proposition 4.1.

The figure 2 presents the numerical approximation $\breve{\zeta}_2(\tau) - 3\breve{\zeta}_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \leqslant k \leqslant 500$. These quantities are positive for $\tau > 0$, therefore we think that $\zeta_2(\tau) - 3\zeta_1(\tau)$ is positive for all $\tau > 0$. Using Proposition 4.6, we believe that the conjecture 4.7 is true.

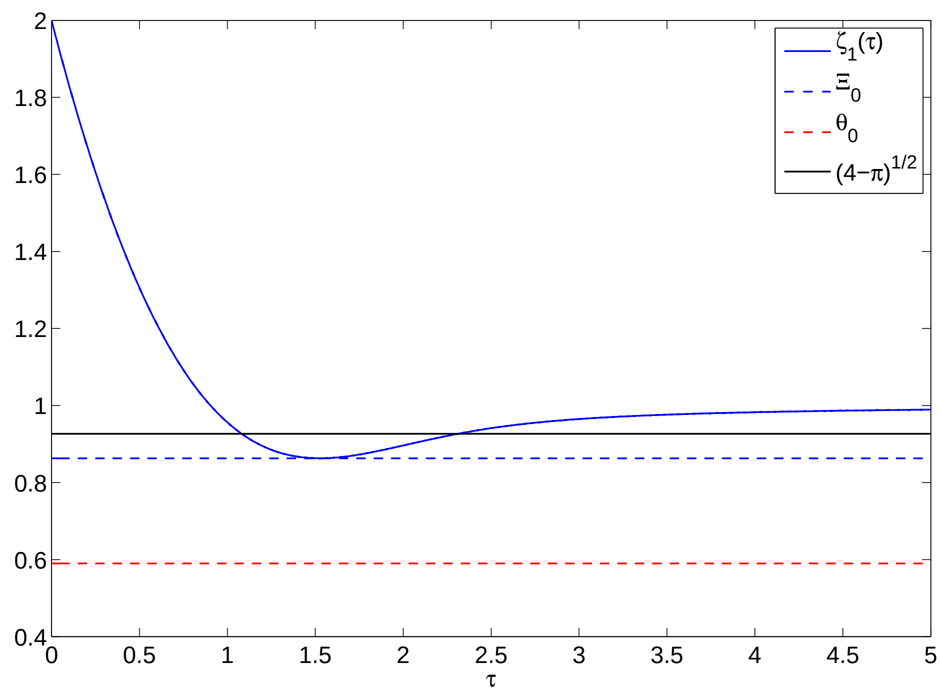

Figure 1. The numerical approximations $\breve{\zeta}_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \leqslant k \leqslant 500$ compared to the constant Θ_0 and the upper bound $\sqrt{4-\pi}$.

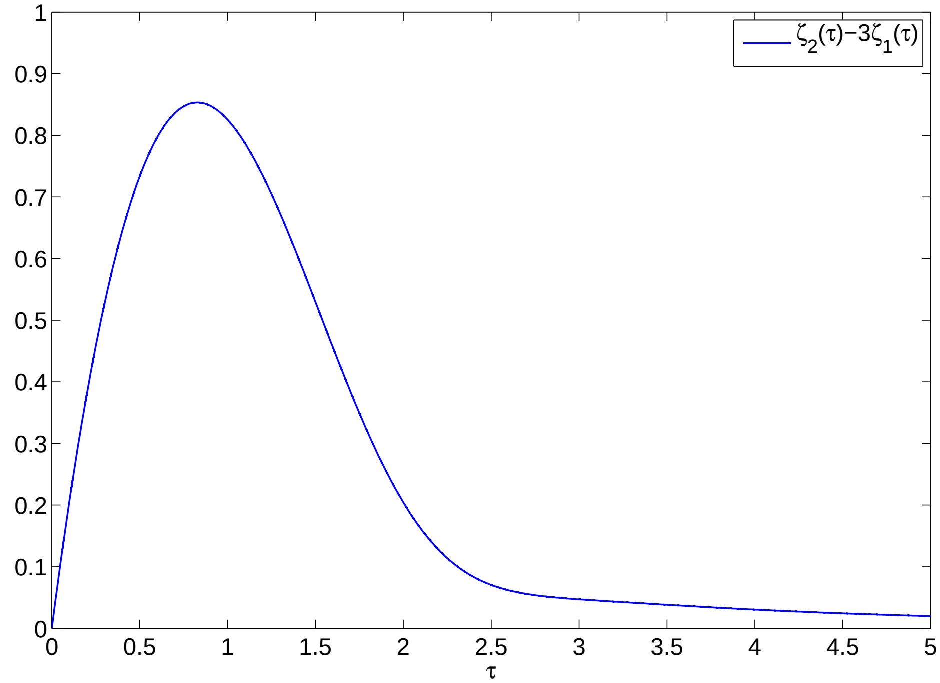

FIGURE 2. The numerical approximations $\breve{\zeta}_2(\tau) - 3\breve{\zeta}_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \leqslant k \leqslant 500$.

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